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Physics-based adaptive learning to resolve overlapping molecular line transitions in mid-infrared spectroscopy

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Mid-Infrared laser-based sensing using molecular spectroscopy is commonly used for trace-gas detection and density measurements. An obvious advantage in detection in the mid-IR region is the fundamental absorption bands of several molecular species of interest for environmental, biomedical, and industrial processing applications. Several challenges in mid-IR sensing are due to significant interference and overlapping line transitions of molecular species with broad collision linewidths. Therefore, in many instances, the absorption signal is congested, overlapping line transitions of disparate molecular oscillator linestrenghts. In this project, we show a novel experimental methodology integrated with adaptive learning techniques to discriminate, quantify and resolve overlapping line transitions of nitrous oxide, water vapor, and methane in the spectral region of 4 um to 10 um. The trace gas detection and machine learning-based classification method utilize the structural complexity of higher harmonic wavelength modulation spectroscopy signals that encode molecular collision dynamics information.

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